

Unified description of ${}^6\text{Li}$ structure and deuterium- ${}^4\text{He}$ dynamics with chiral two- and three-nucleon forces

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Prototype for the study of weakly bound projectiles colliding on stable targets, the scattering of deuterium (d) on ${}^4\text{He}$ (α) is an important milestone in the search for a fundamental understanding of low-energy reactions. At the same time, it is also important for its role in the Big-bang nucleosynthesis of ${}^6\text{Li}$ and applications in the characterization of deuterium impurities in materials. We present the first unified *ab initio* study of the ${}^6\text{Li}$ ground state and d - ${}^4\text{He}$ elastic scattering using two- and three-nucleon forces derived within the framework of chiral effective field theory. The six-nucleon bound-state and scattering observables are calculated by means of the no-core shell model with continuum. We analyze the influence of the dynamic polarization of the deuterium and of the chiral three-nucleon force, and examine the role of the continuum degrees of freedom in shaping the low-lying spectrum of ${}^6\text{Li}$. We find that the adopted Hamiltonian correctly predicts the binding energy of ${}^6\text{Li}$, yielding an asymptotic D - to S -state ratio of the ${}^6\text{Li}$ wave function in $d + \alpha$ configuration of -0.027 in agreement with the value determined from a phase shift analysis of ${}^6\text{Li} + {}^4\text{He}$ elastic scattering, but overestimates the excitation energy of the first 3^+ state by 350 keV. The bulk of the computed differential cross section is in good agreement with data.

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Introduction. Lithium-6 (${}^6\text{Li}$) is a weakly-bound stable nucleus that breaks into an ${}^4\text{He}$ (or α particle) and a deuteron (d) at the excitation energy of 1.4743 MeV [1]. Until now out of reach of *ab initio* (i.e., from first principles) techniques, a complete unified treatment of the bound and continuum properties of this system is desirable to further our understanding of the fundamental interactions among nucleons, but also to inform the evaluation of low-energy cross sections relevant to applications. Notable examples are the ${}^2\text{H}(\alpha, \gamma){}^6\text{Li}$ radiative capture (responsible for the Big-bang nucleosynthesis of ${}^6\text{Li}$ [2–6]) and the ${}^2\text{H}(\alpha, d){}^4\text{He}$ cross section used in the characterization of deuteron concentrations in thin films [7–9]. Contrary to the lighter nuclei, the structure of the ${}^6\text{Li}$ ground state (g.s.) – namely the amount of D -state component in its $d + \alpha$ configuration – is still uncertain [1]. Well known experimentally, the low-lying resonances of ${}^6\text{Li}$ have been shown to present significant sensitivity to three-nucleon ($3N$) interactions in *ab initio* calculations that treated them as bound states [10–13]. However, this approximation is well justified only for the narrow 3^+ first excited state, and no information about the widths was provided. At the same time, the only *ab initio* study of d - ${}^4\text{He}$ scattering [14] was based on a nucleon-nucleon (NN) Hamiltonian and did not take into account the swelling of the α particle due to the interaction with the deuteron.

As demonstrated in a study of the unbound ${}^7\text{He}$ nucleus, the *ab initio* no-core shell model with continuum (NCSMC) [15] is an efficient many-body approach to nuclear bound and scattering states alike. Initially developed to compute nucleon-nucleus collisions starting from a two-body Hamiltonian, this technique has been later extended to include $3N$ forces and successfully applied

to make predictions of elastic scattering and recoil of protons off ${}^4\text{He}$ [16] and to study continuum and $3N$ -force effects on the energy levels of ${}^9\text{Be}$ [17]. We have now developed the NCSMC formalism to describe more challenging deuterium-nucleus collisions, and as a first application, we present in this Letter a study of the ${}^6\text{Li}$ ground state and d - ${}^4\text{He}$ elastic scattering using $NN + 3N$ forces from chiral effective field theory [18, 19].

Approach. We cast the microscopic ansatz for the ${}^6\text{Li}$ wave function in the form of a generalized cluster expansion

$$|\Psi^{J^\pi T}\rangle = \sum_{\lambda} c_{\lambda} |{}^6\text{Li } \lambda J^\pi T\rangle + \sum_{\nu} \int dr r^2 \frac{\gamma_{\nu}(r)}{r} \mathcal{A}_{\nu} |\Phi_{\nu r}^{J^\pi T}\rangle, \quad (1)$$

where J, π and T are respectively total angular momentum, parity and isospin, $|{}^6\text{Li } \lambda J^\pi T\rangle$ represent square-integrable energy eigenstates of the ${}^6\text{Li}$ system, and

$$|\Phi_{\nu r}^{J^\pi T}\rangle = \left[(|{}^4\text{He } \lambda_{\alpha} J_{\alpha}^{\pi_{\alpha}} T_{\alpha}\rangle |{}^2\text{H } \lambda_d J_d^{\pi_d} T_d\rangle)^{(sT)} Y_{\ell}(\hat{r}_{\alpha,d}) \right]^{(J^\pi T)} \times \frac{\delta(r - r_{\alpha,d})}{rr_{\alpha,d}} \quad (2)$$

are continuous basis states built from a ${}^4\text{He}$ and a ${}^2\text{H}$ nuclei whose centers of mass are separated by the relative coordinate $\vec{r}_{\alpha,d}$, and that are moving in a $2^{s+1}\ell_J$ partial wave of relative motion. The translationally-invariant compound, target and projectile states (with energy labels $\lambda, \lambda_{\alpha}$ and λ_d , respectively) are all obtained by means of the no-core shell model (NCSM) [20, 21] using a basis of many-body harmonic oscillator (HO) wave functions with frequency $\hbar\Omega$ and up to N_{max} HO quanta above the lowest energy configuration. The index ν collects the

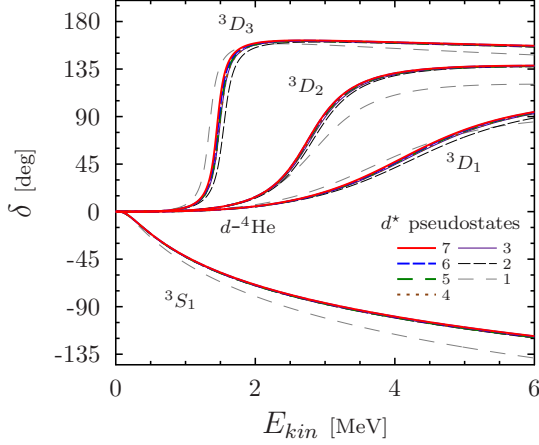


FIG. 1. (Color online) Computed d - ${}^4\text{He}$ S - and D -wave phase shifts at $N_{\text{max}} = 9$ and $\hbar\Omega = 20$ MeV, obtained fifteen square-integrable ${}^6\text{Li}$ eigenstates, as a function of the number of ${}^2\text{H}$ pseudostates (up to seven) in each of the 3S_1 - 3D_1 , 3D_2 and 3D_3 - 3G_3 channels. The two-body part of the SRG-evolved $N^3\text{LO}$ NN potential (NN -only) with $\Lambda = 2.0 \text{ fm}^{-1}$ was used.

quantum numbers $\{{}^4\text{He} \lambda_\alpha J_\alpha^{\pi_\alpha} T_\alpha; {}^2\text{H} \lambda_d J_d^{\pi_d} T_d; s\ell\}$ associated with the continuous basis states of Eq. (2), and the operator (with $P_{i,j}$ exchanging particles i and j)

$$\mathcal{A}_\nu = \frac{1}{\sqrt{15}} \left(1 - \sum_{i=1}^4 \sum_{j=5}^6 P_{i,j} + \sum_{i<j=1}^4 P_{i,5} P_{j,6} \right),$$

ensures its full antisymmetrization. Finally, the unknown discrete coefficients, c_λ , and continuous amplitudes of relative motion, $\gamma_\nu(r)$, are obtained by solving the six-body Schrödinger equation in the Hilbert space spanned by the basis states $|{}^6\text{Li} \lambda J^\pi T\rangle$ and $\mathcal{A}_\nu |\Phi_{\nu r}^{J^\pi T}\rangle$ [15]. The bound state and the elements of the scattering matrix are then obtained from matching the solutions of Eq. (1) with the known asymptotic behavior of the wave function using an extension of the microscopic R -matrix theory [22, 23].

The deuteron is only bound by 2.224 MeV. For relative kinetic energies (E_{kin}) above this threshold, the d - ${}^4\text{He}$ scattering problem is of a three-body nature (until the breakup of the tightly bound ${}^4\text{He}$, that is). Below, the virtual scattering to the energetically closed ${}^4\text{He}+p+n$ channels accounts for the distortion of the projectile. Here we address this by discretizing the continuum of ${}^2\text{H}$ in the 3S_1 - 3D_1 , 3D_2 and 3D_3 - 3G_3 channels identified in our earlier study of Ref. [14]. At the same time, fifteen (among which two 1^+ , two 2^+ , and one 3^+) square-integrable six-body eigenstates of ${}^6\text{Li}$ also contribute to the description of the deuteron distortion. More importantly, they address the swelling of the α particle [16], of which we only include the g.s. in Eq. (2). The typical convergence behavior of our computed d - ${}^4\text{He}$ phase shifts with respect to the number of deuteron pseudostates (or d^* , with $E_{d^*} > 0$) included in Eq. (2) is shown in Fig. 1.

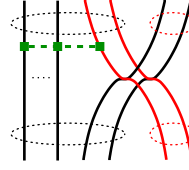


FIG. 2. (Color online) Diagrammatic representation of one of the $3N$ -force matrix elements between basis states of Eq. (2).

Stable results are found with as little as three deuteron pseudostates per channel. This is a strong reduction of the d^* influence with respect to the more limited study of Ref. [14], lacking the coupling of square-integrable ${}^6\text{Li}$ eigenstates. Nonetheless, above the ${}^2\text{H}$ breakup threshold, our approach is approximated and a rigorous treatment would require the more complicated task of including three-cluster basis states [24] in the ansatz of Eq. (1).

The treatment of $3N$ forces within the NCSMC formalism to compute deuteron-nucleus collisions involves major technical and computational challenges. The first is the derivation and calculation of the matrix elements between the continuous basis states of Eq. (2) of seven independent $3N$ -force terms, five of which involve the exchange of one or two nucleons belonging to the projectile with those of the target. A typical example is the diagram of Fig. 2, which for the present application corresponds to $\langle \Phi_{\nu' r'}^{J^\pi T} | P_{3,5} P_{4,6} V_{123}^{3N} | \Phi_{\nu r}^{J^\pi T} \rangle$, with V_{123}^{3N} the $3N$ interaction among particles 1, 2 and 3. To calculate this contribution, we need the four-nucleon density matrix of the target. For ${}^4\text{He}$, this can be precomputed and stored in a factorized form [14, 25]. An additional difficulty is represented by the exorbitant number of input $3N$ -force matrix elements (see Fig. 1 of Ref. [26]), which we have to limit by specifying a maximum three-nucleon HO model space size $E_{3\text{max}}$ [25]. To minimize the effects of such truncation we included $3N$ -force matrix elements up to $E_{3\text{max}} = 17$. The $\langle {}^6\text{Li} \lambda J^\pi T | V_{346}^{3N} | \Phi_{\nu r}^{J^\pi T} \rangle$ and $\langle {}^6\text{Li} \lambda J^\pi T | V_{456}^{3N} | \Phi_{\nu r}^{J^\pi T} \rangle$ couplings between discrete and continuous states are comparatively less demanding.

Results. We adopt an Hamiltonian based on the chiral $N^3\text{LO}$ NN interaction of Ref. [29] and $N^2\text{LO}$ $3N$ force of Ref. [30], constrained to provide an accurate description of the $A=2$ and 3 [31] systems. These interactions are additionally softened by means of a unitary transformation that decouples high- and low-momentum components of the Hamiltonian, working within the similarity renormalization group (SRG) method [26, 32–35]. To minimize the occurrence of induced four-nucleon forces, we work with the SRG momentum scale $\Lambda = 2.0 \text{ fm}^{-1}$ [25, 34, 35]. All calculations are carried out using the ansatz of Eq. (1) with fifteen discrete eigenstates of the ${}^6\text{Li}$ system and continuous d - ${}^4\text{He}$ (g.s.) binary-cluster states with up to seven deuteron pseudostates in the 3S_1 - 3D_1 , 3D_2 and 3D_3 - 3G_3 channels. Similar to our earlier study of d - ${}^4\text{He}$ scattering [14] [performed with a softer NN interaction but in a model space spanned only by the continuous basis states of Eq. (2)], we approach

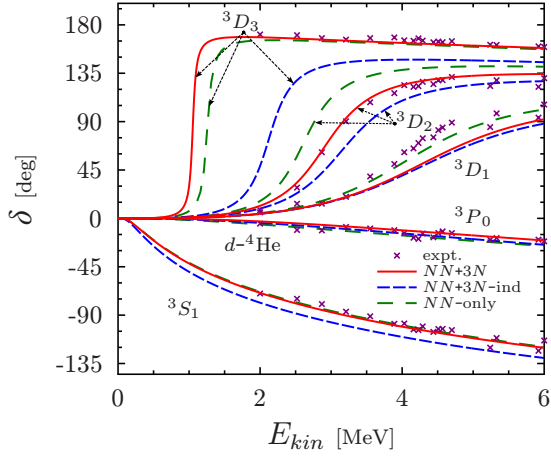


FIG. 3. (Color online) S -, 3P_0 - and D -wave d - ${}^4\text{He}$ phase shifts computed with the NN -only, $NN+3N$ -ind and $NN+3N$ Hamiltonians (lines) compared to those extracted from R -matrix analyses of data [27, 28] (symbols). More details in the text.

convergence for the HO expansions at $N_{\text{max}} = 11$. We adopt the HO frequency of 20 MeV around which the ${}^6\text{Li}$ g.s. energy calculated within the square-integrable basis of the NCSM becomes nearly insensitive to $\hbar\Omega$ [13].

We start by discussing the influence of $3N$ forces – those induced by the SRG transformation of the NN potential ($NN+3N$ -ind) as well as those initially present in the chiral Hamiltonian ($NN+3N$). In Fig. 3 we compare our computed d - ${}^4\text{He}$ S -, 3P_0 - and D -wave phase shifts with those of the R -matrix analyses of Refs. [27, 28]. The results based on the two-body part of the evolved NN force (NN -only) resemble those obtained with a softer potential [14]. Once the SRG unitary equivalence is restored via the induced $3N$ force, the resonance centroids are systematically shifted to higher energies. By contrast, the agreement with data is much improved in the $NN+3N$ case and, in particular, the splitting between the 3D_3 and 3D_2 partial waves is comparable to the measured one.

In Fig. 4, the resonance centroids and widths extracted [36] from the phase shifts of Fig. 3 (shown on the right) are compared with experiment as well as with more traditional approximated energy levels (shown on the left) obtained within the NCSM by treating the ${}^6\text{Li}$ excited states as bound states. In terms of excitation energies relative to the g.s., in both calculations (i.e., with or without continuum effects) the chiral $3N$ force affects mainly the splitting between the 3^+ and 2^+ states, and to a lesser extent the position of the first excited state. Sensitivity to the chiral $3N$ force is also seen in the widths of the NCSMC resonances, which tend to become narrower (in closer agreement with experiment) when this force is present in the initial Hamiltonian. Overall, the closest agreement with the observed spectrum is obtained

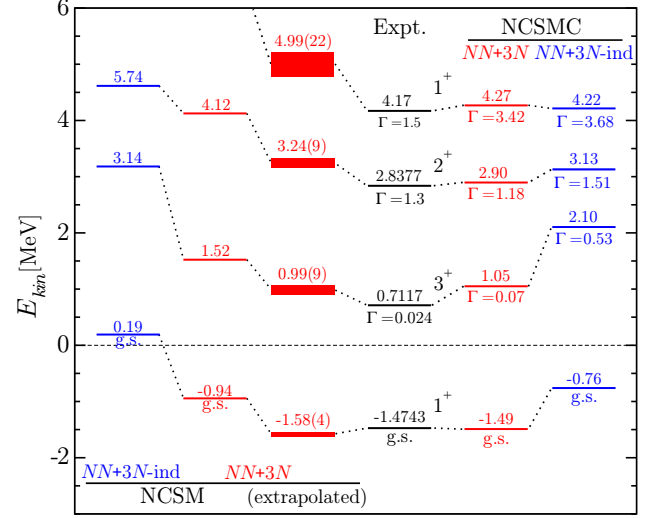


FIG. 4. (Color online) Ground-state energy and low-lying ${}^6\text{Li}$ positive-parity $T = 0$ resonance parameters extracted [36] from the phase shifts of Fig. 3 (NCSMC) compared to the evaluated centroids and widths (indicated by Γ) of Ref. [1] (Expt.). Also shown on the left-hand-side are the best ($N_{\text{max}} = 12$) and extrapolated [37] NCSM energy levels. The zero energy is set to the respective computed (experimental) d - ${}^4\text{He}$ breakup thresholds.

with the $NN+3N$ Hamiltonian working within the NCSMC, i.e. by including the continuum degrees of freedom. Compared to the best ($N_{\text{max}} = 12$) NCSM values, all resonances are shifted to lower energies commensurately with their distance from the d - ${}^4\text{He}$ breakup threshold. For the 3^+ , which is a narrow resonance, the effect is not sufficient to correct for the slight overestimation in excitation energy already observed in the NCSM calculation. This and the ensuing underestimation of the splitting between the 2^+ and 3^+ states point to remaining deficiencies in the adopted $3N$ force model, particularly

TABLE I. Absolute ${}^6\text{Li}$ g.s. energy, S - (C_0) and D -wave (C_2) asymptotic normalization constants and their ratio using the $NN + 3N$ Hamiltonian compared to experiment. Indicated in parenthesis is the N_{max} value of the respective calculation. The error estimates quoted in the extrapolated (∞) NCSM results include uncertainties due to the SRG evolution of the Hamiltonian and $\hbar\Omega$ dependence [13].

Ground-State Properties	$E_{\text{g.s.}}$ [MeV]	C_0 [$\text{fm}^{-1/2}$]	C_2 [$\text{fm}^{-1/2}$]	C_2/C_0
NCSM (10)	-30.84	—	—	—
NCSM (12)	-31.52	—	—	—
NCSM (∞) [37]	-32.2(3)	—	—	—
NCSMC (10)	-32.01	2.695	-0.074	-0.027
Expt.[1, 39, 40]	-31.99	2.91(9)	-0.077(18)	-0.025(6)(10)
Expt. [38, 41]	—	2.93(15)	—	0.0003(9)

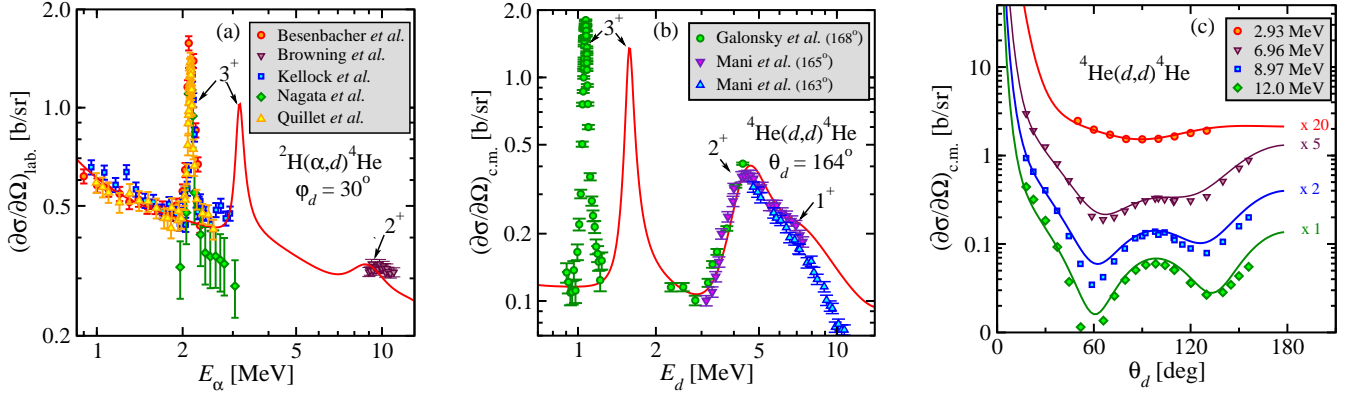


FIG. 5. (Color online) Computed (a) $^2\text{H}(\alpha, d)^4\text{He}$ laboratory-frame and (b) $^4\text{He}(d, d)^4\text{He}$ center-of-mass frame angular differential cross sections (lines) using the $NN+3N$ Hamiltonian at the deuteron recoil and backscattered angles of, respectively, $\varphi_d = 30^\circ$ and $\theta_d = 164^\circ$ as a function of the laboratory helium (E_α) and deuteron (E_d) incident energies, compared with data (symbols) from Refs. [7–9, 42–45]. In panel (c), calculated (lines) and measured (symbols) center-of-mass angular distributions at $E_d = 2.93, 6.96, 8.97$ [46], and 12 MeV [47] are scaled by a factor of 20, 5, 2, and 1, respectively. All positive- and negative-parity partial waves up to $J = 3$ were included in the calculations.

concerning the strength of the spin-orbit interaction.

The inclusion of the $d+^4\text{He}$ states of Eq. (2) results also in additional binding for the 1^+ ground state. This stems from a more efficient description of the clusterization of ^6Li into $d+\alpha$ at long distances, which is harder to describe within a finite HO model space, or – more simply – from the increased size of the many-body model space. Indeed, as shown in Fig. 4 and in Table I for the absolute value of the ^6Li g.s. energy, extrapolating to $N_{\text{max}} \rightarrow \infty$ [37] brings the NCSM results in good agreement with the NCSMC, particularly for bound states and narrow resonances. However, while the extrapolation procedure yields comparable energies, only the NCSMC wave functions present the correct asymptotic, which for the g.s. is a Whittaker function. This is essential for the extraction of the asymptotic normalization constants and a future description of the $^2\text{H}(\alpha, \gamma)^6\text{Li}$ radiative capture [5]. The obtained asymptotic D - to S -state ratio is not compatible with the near zero value of Ref. [41], but rather is in good agreement with the determination of Ref. [39], stemming from an analysis of $^6\text{Li}+^4\text{He}$ elastic scattering. Further, based on the extrapolated NCSM energies, one could erroneously conclude that the measured splitting between 2^+ and 3^+ state is reproduced with the $NN+3N$ Hamiltonian. Conversely, the square-integrable $|\ ^6\text{Li} \lambda J^\pi T \rangle$ components of Eq. (1) are key to achieving an efficient description of the short-range six-body correlations, and compensate for computationally arduous to include ^4He excited states.

Next, in Figs. 5(a) and 5(b), respectively, we compare the $^2\text{H}(\alpha, d)^4\text{He}$ deuteron elastic recoil and $^4\text{He}(d, d)^4\text{He}$ deuteron elastic scattering differential cross sections computed using the $NN+3N$ Hamiltonian to the measured energy distributions of Refs. [7–9, 42–45]. Aside from the position of the 3^+ resonance, the calculations are in fair agreement with experiment, particularly in the low-

energy region of interest for the Big-bang nucleosynthesis of ^6Li , where we reproduce the data of Besenbacher *et al.* [42] and those of Quillet *et al.* [8]. The 500 keV region below the resonance in Fig. 5(a) is also important for material science, where the elastic recoil of deuterium knocked by incident α particles is used to analyze the presence of this element. At higher energies, near the 2^+ and 1^+ resonances, the computed cross section at the center-of-mass deuteron scattering angle of $\theta_d = 164^\circ$ reproduces the data of Galonsky *et al.* [44] and Mani *et al.* [45], while we find slight disagreement with the data of Ref. [9] in the elastic recoil configuration at the laboratory angle of $\varphi_d = 30^\circ$. At even higher energies, the measured cross section of Fig. 5(b) lies below the calculated one. This is due to the overestimated width of the 1_2^+ state, which is twice as large as in experiment. The overall good agreement with experiment is also corroborated by Fig. 5(c), presenting $^4\text{He}(d, d)^4\text{He}$ angular distributions in the $2.93 \leq E_d \leq 12.0$ MeV interval of incident energies. In particular, the theoretical curves reproduce the data at 2.93 and 6.96 MeV, while some deviations are visible at the two higher energies, in line with our previous discussion. Nevertheless, in general the present results with $3N$ forces provide a much more realistic description of the scattering process than our earlier study of Ref. [14]. Finally, we expect that an $N_{\text{max}} = 13$ calculation (currently out of reach) would not significantly change the present picture, particularly concerning the narrow 3^+ resonance. Indeed, much as in the case of the g.s. energy, here the NCSMC centroid is in good agreement with the NCSM extrapolated value, 0.99(9) MeV.

Conclusions. We presented the first application of the *ab initio* NCSMC formalism to the description of deuteron-nucleus dynamics. We illustrated the role of the chiral $3N$ force and continuous degrees of freedom in determining the bound-state properties of ^6Li and $d\text{-}^4\text{He}$

elastic scattering observables. The computed g.s. energy is in excellent agreement with experiment, and our $d+\alpha$ asymptotic normalization constants support a non-zero negative ratio of D - to S -state components for ${}^6\text{Li}$. We used data for deuterium backscattering and recoil cross sections of interests to ion beam spectroscopy to validate our scattering calculations and found a good agreement in particular at low energy. The overestimation by about 350 keV of the position of the 3^+ resonance is an indication of remaining deficiencies of the nuclear Hamiltonian employed here. This work sets the stage for the first *ab initio* study of the ${}^2\text{H}(\alpha, \gamma){}^6\text{Li}$ radiative capture, and is a stepping stone in the calculation of the deuterium-tritium fusion with the chiral $NN + 3N$ Hamiltonian, currently in progress.

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